MSG No. 191.234 $P6/mmm1'$ [Type II, hexagonal]

Table 1: Wyckoff site: 1a, site symmetry: 6/mmm1'

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,
		25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]

Table 2: Wyckoff site: 1b, site symmetry: 6/mmm1'

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,
		25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]

Table 3: Wyckoff site: 2c, site symmetry: -6m21'

No.	position	mapping
1	$\left[\frac{1}{3}, \frac{2}{3}, 0\right]$	[1,3,5,10,11,12,14,16,18,19,20,21,25,27,29,34,35,36,38,40,42,43,44,45]
2	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	[2,4,6,7,8,9,13,15,17,22,23,24,26,28,30,31,32,33,37,39,41,46,47,48]

Table 4: Wyckoff site: 2d, site symmetry: -6m21'

No.	position	mapping
1	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}\right]$	[1,3,5,10,11,12,14,16,18,19,20,21,25,27,29,34,35,36,38,40,42,43,44,45]
2	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}\right]$	[2,4,6,7,8,9,13,15,17,22,23,24,26,28,30,31,32,33,37,39,41,46,47,48]

Table 5: Wyckoff site: 2e, site symmetry: 6mm1'

No.	position	mapping
1	$[0, 0, z]$	[1,2,3,4,5,6,19,20,21,22,23,24,25,26,27,28,29,30,43,44,45,46,47,48]
2	$[0, 0, -z]$	[7,8,9,10,11,12,13,14,15,16,17,18,31,32,33,34,35,36,37,38,39,40,41,42]

Table 6: Wyckoff site: 3f, site symmetry: mmm1'

No.	position	mapping
1	$\left[\frac{1}{2}, 0, 0\right]$	[1,4,7,11,13,16,19,23,25,28,31,35,37,40,43,47]
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[2,5,9,10,14,17,21,22,26,29,33,34,38,41,45,46]

continued ...

Table 6

No.	position	mapping
3	$\left[0,\ \frac{1}{2},\ 0\right]$	[3,6,8,12,15,18,20,24,27,30,32,36,39,42,44,48]

Table 7: Wyckoff site: 3g, site symmetry: mmm1'

No.	position	mapping
1	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	[1,4,7,11,13,16,19,23,25,28,31,35,37,40,43,47]
2	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	[2,5,9,10,14,17,21,22,26,29,33,34,38,41,45,46]
3	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	[3,6,8,12,15,18,20,24,27,30,32,36,39,42,44,48]

Table 8: Wyckoff site: 4h, site symmetry: 3m.1'

No.	position	mapping
1	$\left[\frac{1}{3},\ \frac{2}{3},\ z\right]$	[1,3,5,19,20,21,25,27,29,43,44,45]
2	$\left[\frac{2}{3},\ \frac{1}{3},\ z\right]$	[2,4,6,22,23,24,26,28,30,46,47,48]
3	$\left[\frac{2}{3},\ \frac{1}{3},\ -z\right]$	[7,8,9,13,15,17,31,32,33,37,39,41]
4	$\left[\frac{1}{3},\ \frac{2}{3},\ -z\right]$	[10,11,12,14,16,18,34,35,36,38,40,42]

Table 9: Wyckoff site: 6i, site symmetry: 2mm1'

No.	position	mapping
1	$\left[\frac{1}{2},\ 0,\ z\right]$	[1,4,19,23,25,28,43,47]
2	$\left[\frac{1}{2},\ \frac{1}{2},\ z\right]$	[2,5,21,22,26,29,45,46]
3	$\left[0,\ \frac{1}{2},\ z\right]$	[3,6,20,24,27,30,44,48]
4	$\left[\frac{1}{2},\ 0,\ -z\right]$	[7,11,13,16,31,35,37,40]
5	$\left[0,\ \frac{1}{2},\ -z\right]$	[8,12,15,18,32,36,39,42]
6	$\left[\frac{1}{2},\ \frac{1}{2},\ -z\right]$	[9,10,14,17,33,34,38,41]

Table 10: Wyckoff site: 6j, site symmetry: m2m1'

No.	position	mapping
1	$[x,\ 0,\ 0]$	[1,7,16,23,25,31,40,47]
2	$[x,\ x,\ 0]$	[2,10,17,21,26,34,41,45]
3	$[0,\ x,\ 0]$	[3,8,18,24,27,32,42,48]
4	$[-x,\ 0,\ 0]$	[4,11,13,19,28,35,37,43]
5	$[-x,\ -x,\ 0]$	[5,9,14,22,29,33,38,46]
6	$[0,\ -x,\ 0]$	[6,12,15,20,30,36,39,44]

Table 11: Wyckoff site: `6k`, site symmetry: `m2m1'`

No.	position	mapping
1	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[1,7,16,23,25,31,40,47]`
2	$\left[x,\ x,\ \frac{1}{2}\right]$	`[2,10,17,21,26,34,41,45]`
3	$\left[0,\ x,\ \frac{1}{2}\right]$	`[3,8,18,24,27,32,42,48]`
4	$\left[-x,\ 0,\ \frac{1}{2}\right]$	`[4,11,13,19,28,35,37,43]`
5	$\left[-x,\ -x,\ \frac{1}{2}\right]$	`[5,9,14,22,29,33,38,46]`
6	$\left[0,\ -x,\ \frac{1}{2}\right]$	`[6,12,15,20,30,36,39,44]`

Table 12: Wyckoff site: `6l`, site symmetry: `mm21'`

No.	position	mapping
1	$[x,\ 2x,\ 0]$	`[1,11,16,19,25,35,40,43]`
2	$[-x,\ x,\ 0]$	`[2,9,17,22,26,33,41,46]`
3	$[-2x,\ -x,\ 0]$	`[3,12,18,20,27,36,42,44]`
4	$[-x,\ -2x,\ 0]$	`[4,7,13,23,28,31,37,47]`
5	$[x,\ -x,\ 0]$	`[5,10,14,21,29,34,38,45]`
6	$[2x,\ x,\ 0]$	`[6,8,15,24,30,32,39,48]`

Table 13: Wyckoff site: `6m`, site symmetry: `mm21'`

No.	position	mapping
1	$\left[x,\ 2x,\ \frac{1}{2}\right]$	`[1,11,16,19,25,35,40,43]`
2	$\left[-x,\ x,\ \frac{1}{2}\right]$	`[2,9,17,22,26,33,41,46]`
3	$\left[-2x,\ -x,\ \frac{1}{2}\right]$	`[3,12,18,20,27,36,42,44]`
4	$\left[-x,\ -2x,\ \frac{1}{2}\right]$	`[4,7,13,23,28,31,37,47]`
5	$\left[x,\ -x,\ \frac{1}{2}\right]$	`[5,10,14,21,29,34,38,45]`
6	$\left[2x,\ x,\ \frac{1}{2}\right]$	`[6,8,15,24,30,32,39,48]`

Table 14: Wyckoff site: `12n`, site symmetry: `..m1'`

No.	position	mapping
1	$[x,\ 0,\ z]$	`[1,23,25,47]`
2	$[x,\ x,\ z]$	`[2,21,26,45]`
3	$[0,\ x,\ z]$	`[3,24,27,48]`
4	$[-x,\ 0,\ z]$	`[4,19,28,43]`
5	$[-x,\ -x,\ z]$	`[5,22,29,46]`
6	$[0,\ -x,\ z]$	`[6,20,30,44]`
7	$[x,\ 0,\ -z]$	`[7,16,31,40]`
8	$[0,\ x,\ -z]$	`[8,18,32,42]`
9	$[-x,\ -x,\ -z]$	`[9,14,33,38]`

continued ...

Table 14

No.	position	mapping
10	$[x,\ x,\ -z]$	[10,17,34,41]
11	$[-x,\ 0,\ -z]$	[11,13,35,37]
12	$[0,\ -x,\ -z]$	[12,15,36,39]

Table 15: Wyckoff site: 12o, site symmetry: .m.1'

No.	position	mapping
1	$[x,\ 2x,\ z]$	[1,19,25,43]
2	$[-x,\ x,\ z]$	[2,22,26,46]
3	$[-2x,\ -x,\ z]$	[3,20,27,44]
4	$[-x,\ -2x,\ z]$	[4,23,28,47]
5	$[x,\ -x,\ z]$	[5,21,29,45]
6	$[2x,\ x,\ z]$	[6,24,30,48]
7	$[-x,\ -2x,\ -z]$	[7,13,31,37]
8	$[2x,\ x,\ -z]$	[8,15,32,39]
9	$[-x,\ x,\ -z]$	[9,17,33,41]
10	$[x,\ -x,\ -z]$	[10,14,34,38]
11	$[x,\ 2x,\ -z]$	[11,16,35,40]
12	$[-2x,\ -x,\ -z]$	[12,18,36,42]

Table 16: Wyckoff site: 12p, site symmetry: m..1'

No.	position	mapping
1	$[x,\ y,\ 0]$	[1,16,25,40]
2	$[x-y,\ x,\ 0]$	[2,17,26,41]
3	$[-y,\ x-y,\ 0]$	[3,18,27,42]
4	$[-x,\ -y,\ 0]$	[4,13,28,37]
5	$[-x+y,\ -x,\ 0]$	[5,14,29,38]
6	$[y,\ -x+y,\ 0]$	[6,15,30,39]
7	$[x-y,\ -y,\ 0]$	[7,23,31,47]
8	$[y,\ x,\ 0]$	[8,24,32,48]
9	$[-x,\ -x+y,\ 0]$	[9,22,33,46]
10	$[x,\ x-y,\ 0]$	[10,21,34,45]
11	$[-x+y,\ y,\ 0]$	[11,19,35,43]
12	$[-y,\ -x,\ 0]$	[12,20,36,44]

Table 17: Wyckoff site: `12q`, site symmetry: `m..1'`

No.	position	mapping
1	$\left[x,\, y,\, \frac{1}{2}\right]$	`[1,16,25,40]`
2	$\left[x-y,\, x,\, \frac{1}{2}\right]$	`[2,17,26,41]`
3	$\left[-y,\, x-y,\, \frac{1}{2}\right]$	`[3,18,27,42]`
4	$\left[-x,\, -y,\, \frac{1}{2}\right]$	`[4,13,28,37]`
5	$\left[-x+y,\, -x,\, \frac{1}{2}\right]$	`[5,14,29,38]`
6	$\left[y,\, -x+y,\, \frac{1}{2}\right]$	`[6,15,30,39]`
7	$\left[x-y,\, -y,\, \frac{1}{2}\right]$	`[7,23,31,47]`
8	$\left[y,\, x,\, \frac{1}{2}\right]$	`[8,24,32,48]`
9	$\left[-x,\, -x+y,\, \frac{1}{2}\right]$	`[9,22,33,46]`
10	$\left[x,\, x-y,\, \frac{1}{2}\right]$	`[10,21,34,45]`
11	$\left[-x+y,\, y,\, \frac{1}{2}\right]$	`[11,19,35,43]`
12	$\left[-y,\, -x,\, \frac{1}{2}\right]$	`[12,20,36,44]`

Table 18: Wyckoff site: `24r`, site symmetry: `11'`

No.	position	mapping
1	$[x,\, y,\, z]$	`[1,25]`
2	$[x-y,\, x,\, z]$	`[2,26]`
3	$[-y,\, x-y,\, z]$	`[3,27]`
4	$[-x,\, -y,\, z]$	`[4,28]`
5	$[-x+y,\, -x,\, z]$	`[5,29]`
6	$[y,\, -x+y,\, z]$	`[6,30]`
7	$[x-y,\, -y,\, -z]$	`[7,31]`
8	$[y,\, x,\, -z]$	`[8,32]`
9	$[-x,\, -x+y,\, -z]$	`[9,33]`
10	$[x,\, x-y,\, -z]$	`[10,34]`
11	$[-x+y,\, y,\, -z]$	`[11,35]`
12	$[-y,\, -x,\, -z]$	`[12,36]`
13	$[-x,\, -y,\, -z]$	`[13,37]`
14	$[-x+y,\, -x,\, -z]$	`[14,38]`
15	$[y,\, -x+y,\, -z]$	`[15,39]`
16	$[x,\, y,\, -z]$	`[16,40]`
17	$[x-y,\, x,\, -z]$	`[17,41]`
18	$[-y,\, x-y,\, -z]$	`[18,42]`
19	$[-x+y,\, y,\, z]$	`[19,43]`
20	$[-y,\, -x,\, z]$	`[20,44]`
21	$[x,\, x-y,\, z]$	`[21,45]`
22	$[-x,\, -x+y,\, z]$	`[22,46]`
23	$[x-y,\, -y,\, z]$	`[23,47]`
24	$[y,\, x,\, z]$	`[24,48]`